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MEMORANDUM FOR PRS (In-House Publication)

FROM: PROI (STINFO) 22 March 2002

SUBJECT: Authorization for Release of Technical Information, Control Number: **AFRL-PR-ED-VG-2002-068**
Jeff Sheehy, et al. (PRSP), "Computational Chemistry Studies of HEDM"

AF Chief Scientists **(Statement A)**
(Edwards AFB, CA, 07 March 2002) **(Deadline: Past Due)**

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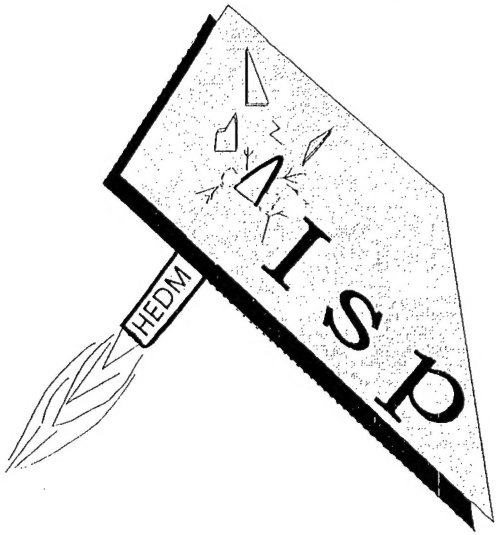
PHILIP A. KESSEL Date
Technical Advisor
Space and Missile Propulsion Division

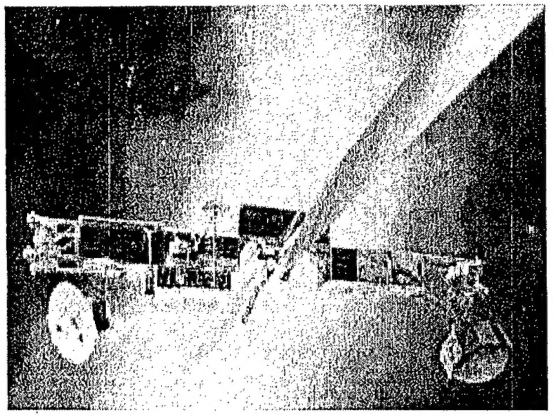
High Energy Density Materials (HEDM) Program Objective

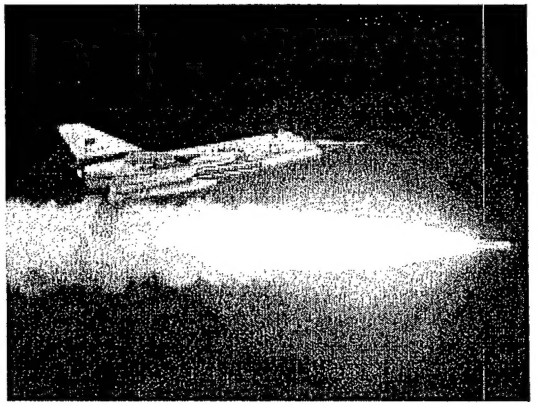


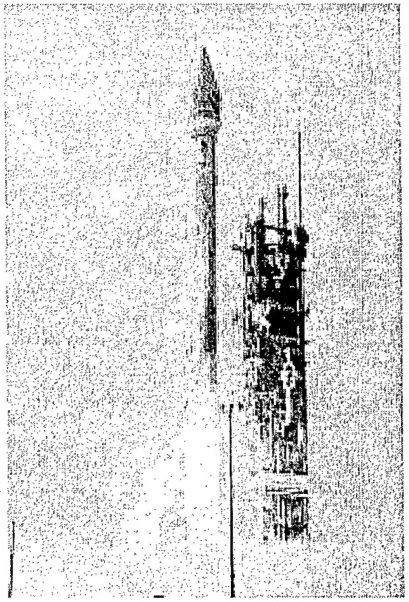
Breaking the performance barrier

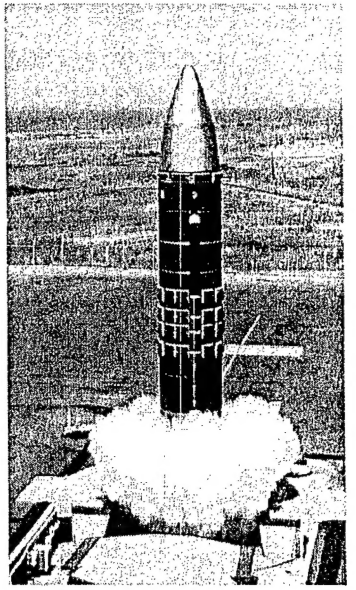
Identify and develop advanced chemical propellants for rocket propulsion applications

- Hydrocarbons for liquid boosters
- Liquid & solid oxidizers for boost and upper stages
- Monopropellants for upper stages and satellites
- Cryogenic propellants for upper stages









HEDM Propellant Payoffs

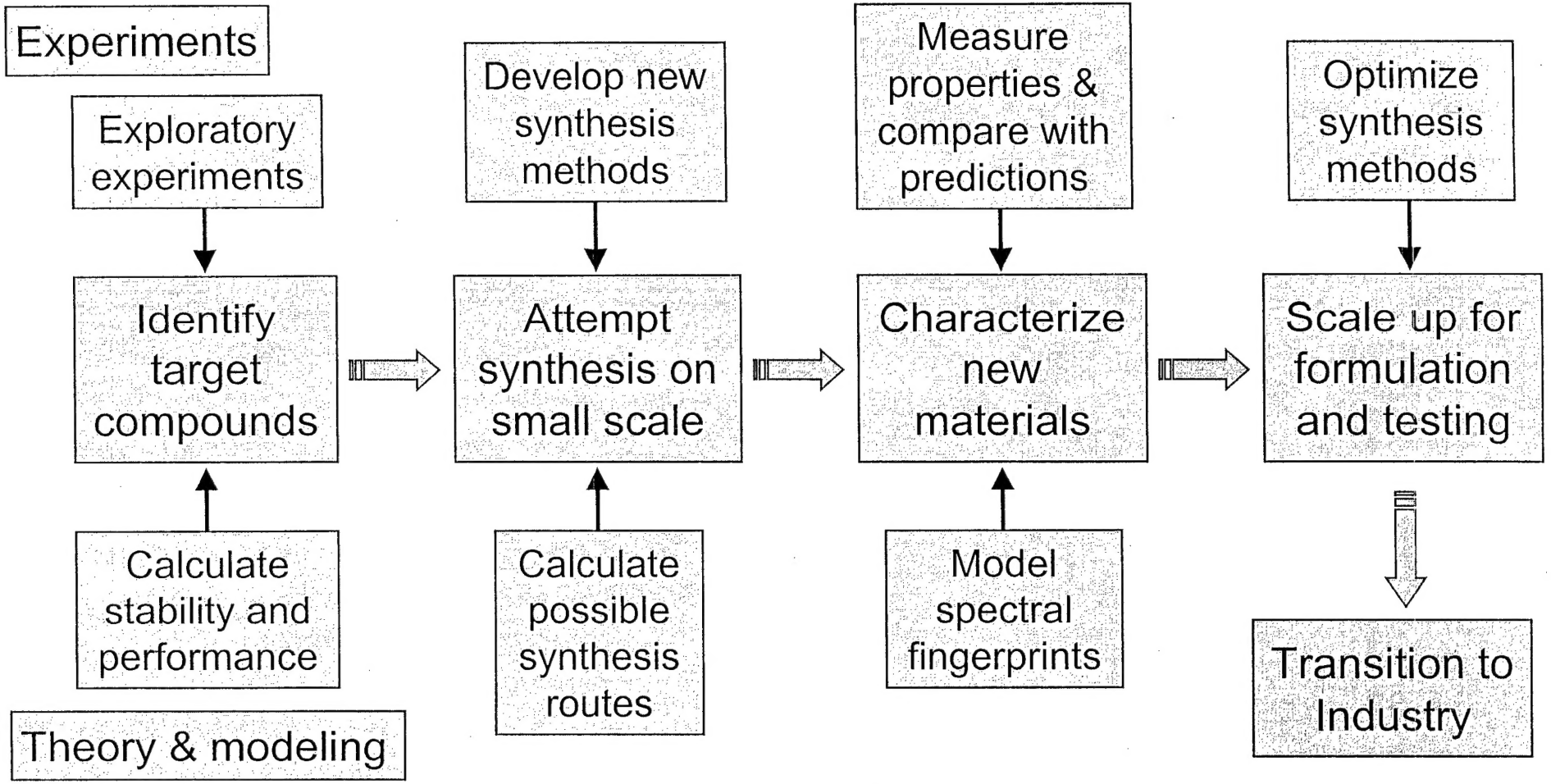
"The highest leverage technology area impacting launch vehicles is the development of high-energy-density materials for use as propellants."
-- New World Vistas Panel on Space Technology (1995)

Vehicle Type	Baseline Vehicle	Propellant	Takeoff Mass (lb)	Payload Mass (lb)	Payload Mass (lb) With 10% Isp Increase
Two-stage ELV	Atlas II // Centaur D-1A	RP-1/LOX (Isp = 295 s) // LH2/LOX (Isp = 455 s)	360,000	12,500	15,600 **(+25%)**
SSTO RLV	Lockheed SSTO	LH2/LOX (Isp = 455 s)	1,900,000	40,000	68,000 **(+70%)**
Missile Defense Interceptor	Boost-Phase Interceptor	HTPB/Al/HMX (Isp = 270 s)	1,847	74	110 **(+49%)**

Our research is aimed at increasing propellant Isp by 5 to 50%

HEDM Program General Approach

Employ a synergic blend of experimental, theoretical, and computational techniques derived from the disciplines of chemistry and physics



The Calculation of Molecular Properties

Various computational techniques are employed to solve the molecular electronic Schrödinger equation from quantum mechanics:

$$\left[-\frac{1}{2}\sum_i \nabla_i^2 - \sum_i \sum_\alpha \frac{Z_\alpha}{r_{i\alpha}} + \sum_i \sum_{j>i} \frac{1}{r_{ij}}\right]\Psi_{el} = E_{el}\Psi_{el}$$

Determining what to synthesize:

Thermodynamic properties relate directly to propellant performance and are obtained from relative energies of reactants, intermediates, and products

Determining how to synthesize them:

Potential-energy surfaces – energy profiles associated with all degrees of freedom in a chemical system – give insight into stabilities and reaction & decomposition pathways

Determining whether we've made what we wanted to make:

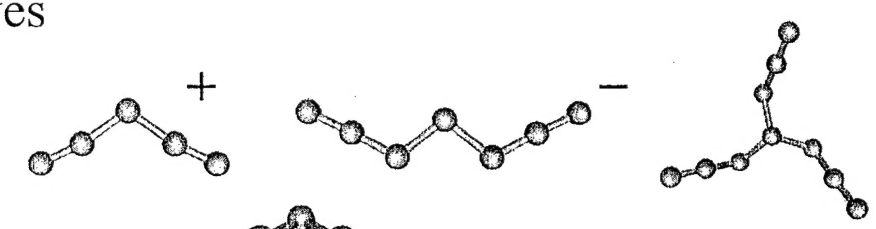
Structures and spectra (IR, Raman, NMR) are obtained by evaluating derivatives of the energy or other properties with respect to nuclear coordinates or applied fields

DARPA Polynitrogen Program

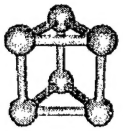
Program began late FY98

Six groups funded to discover, scale up, and demonstrate polynitrogen propellants or explosives

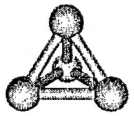
AFRL / Edwards



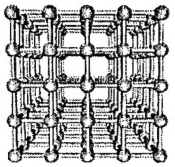
Naval Research Laboratory



Los Alamos National Laboratory

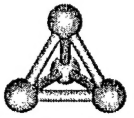


Lawrence Livermore National Laboratory



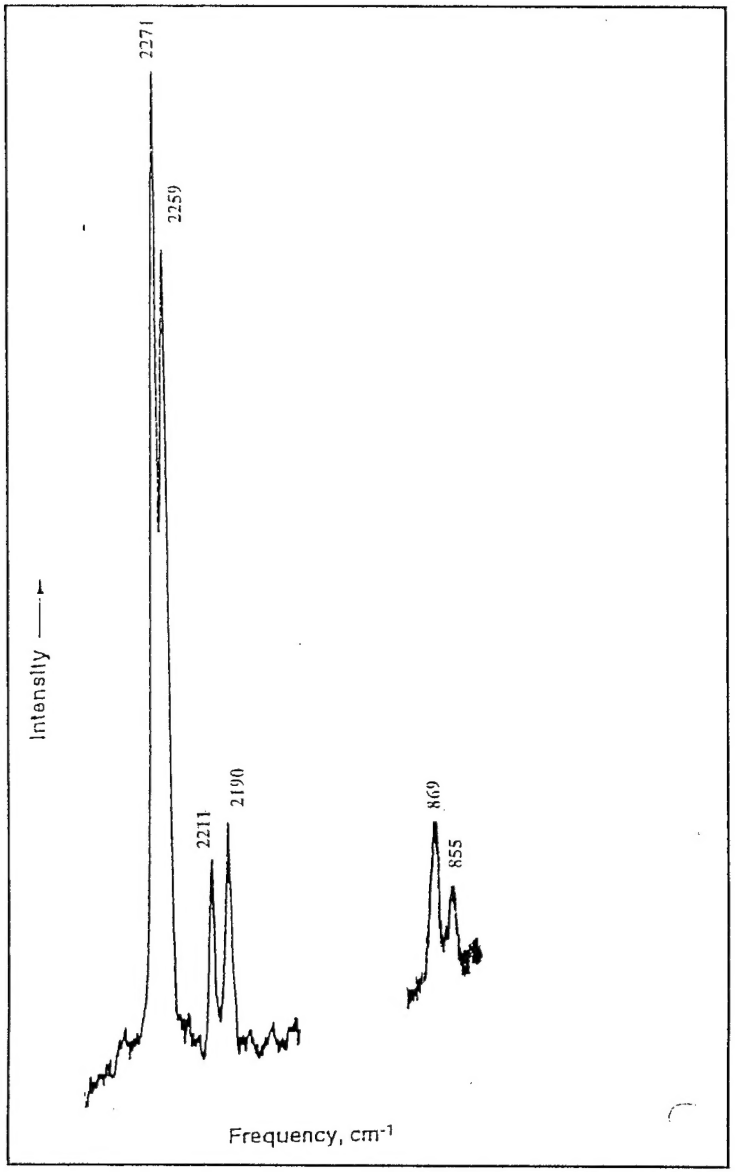
Colorado School of Mines / National Renewable Energy Laboratory

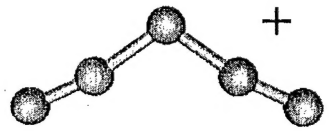
Defense Research Establishment, Sweden



Only the AFRL group has been successful

Identifying a Completely New Molecule: Comparison of Calculated and Measured Spectra





$[^{15}N–^{14}N–^{14}N–^{14}N–^{14}N]^+AsF_6^-$

and

$[^{14}N–^{14}N–^{15}N–^{14}N–^{14}N]^+AsF_6^-$

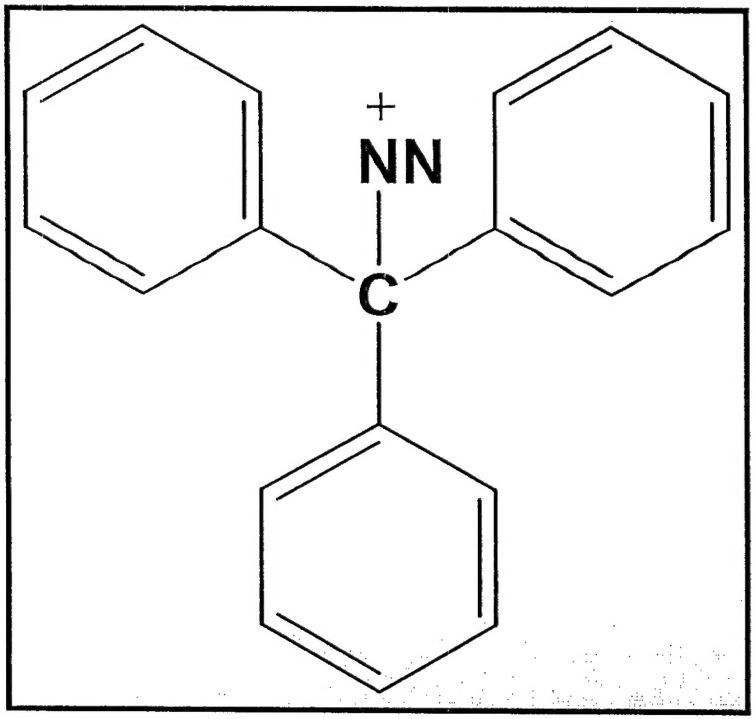
^{14}N - ^{15}N Isotopic Shifts (cm^{-1})

Mode	Obs.	Calc.†
$\nu_1(a_1)$	12	11.8
$\nu_7(b_2)$	21	21.4
$\nu_2(a_1)$	14	14.1

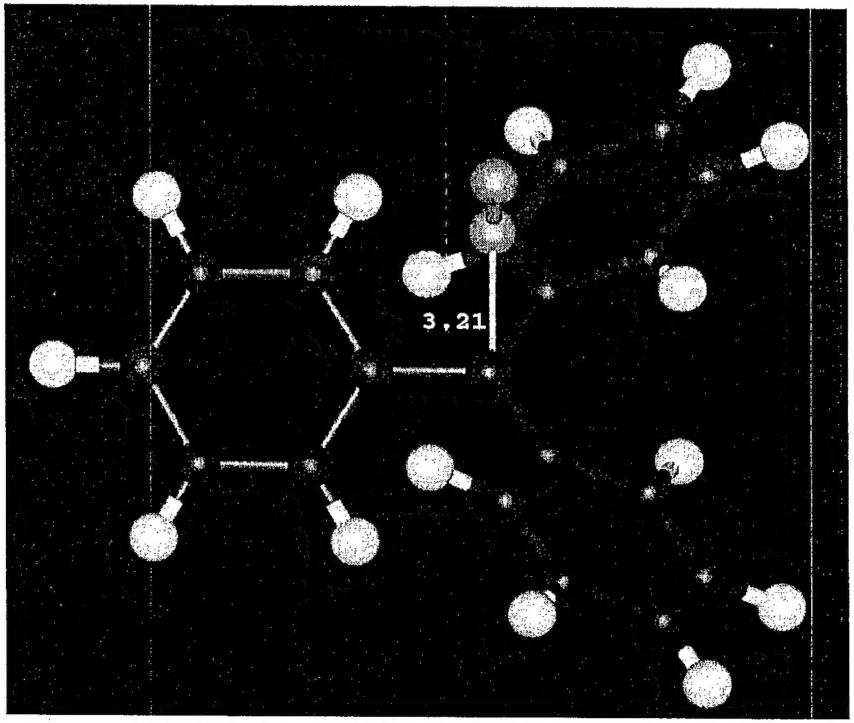
†CCSD(T)/6-311+G(2*d*) results

Identifying Potential Polynitrogen Precursors

This ion has been suggested as a useful precursor to new polynitrogen molecules...



... but calculations predict it to be unstable.



Summary

Computational chemistry plays a critical role in HEDM research

Guides the choice of target compounds and possible synthetic routes, provides verification of successful synthesis.

CC is addressing an ever wider range of Air Force applications

New methods are under development (e.g., modeling chemistry in solution or on surfaces). Parallel computing technology has greatly expanded the scope of problems which can be modeled.

Access to high performance computing resources is essential

Many quantum chemical calculations are too costly and complex to perform on "standard" platforms (e.g., standalone workstations or desktop Linux PCs).